

# Position-momentum uncertainty relations based on moments of arbitrary order

Steeve Zozor,<sup>1</sup> Mariela Portesi,<sup>2</sup> Pablo Sanchez-Moreno,<sup>3,4</sup> and Jesus S. Dehesa<sup>5,6</sup>

<sup>1</sup>*Laboratoire Grenoblois d'Image, Parole,*

*Signal et Automatique (GIPSA-Lab,*

*CNRS), 961 rue de la Houille Blanche,*

*F-38402 Saint Martin d'Hères, France\**

<sup>2</sup>*Instituto de Física La Plata (CONICET),*

*and Departamento de Física, Facultad de Ciencias Exactas,*

*Universidad Nacional de La Plata, 1900 La Plata, Argentina†*

<sup>3</sup>*Instituto Carlos I de Física Teórica y Computacional,*

*Universidad de Granada, 18071-Granada, Spain*

<sup>4</sup>*Departamento de Matemática Aplicada,*

*Universidad de Granada, E-18071 Granada, Spain‡*

<sup>5</sup>*Instituto Carlos I de Física Teórica y Computacional,*

*Universidad de Granada, E-18071 Granada, Spain*

<sup>6</sup>*Departamento de Física Atómica, Molecular y Nuclear,*

*Universidad de Granada, E-18071 Granada, Spain§*

## Abstract

The position-momentum uncertainty-like inequality based on moments of arbitrary order for  $d$ -dimensional quantum systems, which is a generalization of the celebrated Heisenberg formulation of the uncertainty principle, is improved here by use of the Rényi-entropy-based uncertainty relation. The accuracy of the resulting lower bound is physico-computationally analyzed for the two main prototypes in  $d$ -dimensional physics: the hydrogenic and oscillator-like systems.

PACS numbers: 03.65.Ca, 02.50.-r, 05.90.+m, 03.65.Ta

Keywords: Position-momentum uncertainty relation, Rényi entropy,  $d$ -dimensional quantum physics, hydrogenic atoms, oscillator-like systems.

---

\* steeve.zozor@gipsa-lab.grenoble-inp.fr

† portesi@fisica.unlp.edu.ar

‡ pablos@ugr.es

§ dehesa@ugr.es

## I. INTRODUCTION

The uncertainty relations play a fundamental role not only in the foundations of quantum mechanics [1, 2] but also for the quantum description of the internal structure of  $d$ -dimensional physical systems [1–5] as well as for the development of quantum information and computation [6, 7]. The (position-momentum) uncertainty principle has attracted considerable attention since the early days of quantum mechanics [8, 9] up until now [1, 2, 10–12] because of its numerous scientific and technological implications. The first mathematical relation which expresses this principle in an exact and quantitative form is the celebrated Heisenberg relation [8, 9] which uses the standard deviation or its square, the variance of position and momentum, as measure of uncertainty; assuming  $\langle \mathbf{x} \rangle = \langle \mathbf{p} \rangle = 0$  for notational simplicity, it reads as

$$\langle r^2 \rangle \langle p^2 \rangle \geq \frac{d^2}{4} \quad (1)$$

for  $d$ -dimensional quantum-mechanical states.

However, this relation is not only too weak but also it is often inadequate [12–16]. In order to take care of these problems, various alternative formulations of the uncertainty principle have been proposed by use of some information-theoretic uncertainty measures like the Shannon entropy [17], Rényi entropies [18–20], Tsallis entropies [21, 22], entropic momenta [23] and Fisher information [24–26], as recently surveyed [5, 12, 27].

Not so well known is the moment-based uncertainty relation developed by Angulo [28, 29] in 1993 which can be recast [5] under the form

$$\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geq \mathcal{D}(a, b) = \left( \frac{e d^{\frac{2}{a}} \Gamma^{\frac{2}{d}} (1 + \frac{d}{2})}{(ae)^{\frac{2}{a}} \Gamma^{\frac{2}{d}} (1 + \frac{d}{a})} \right) \left( \frac{e d^{\frac{2}{b}} \Gamma^{\frac{2}{d}} (1 + \frac{d}{2})}{(be)^{\frac{2}{b}} \Gamma^{\frac{2}{d}} (1 + \frac{d}{b})} \right) \quad (2)$$

valid for all  $(a, b) \in \mathbb{R}_+^2 = (0, +\infty)^2$ . This relation, which offers a more general and versatile formulation of the uncertainty principle (note that it reduces to the Heisenberg inequality (1) in the particular case  $a = b = 2$ ), has not received so much attention despite the knowledge of the moments often completely characterize a probability density. Strictly speaking, in the  $d$ -dimensional case and when the characteristic function admits a Taylor expansion at any order, the assertion that the moments characterize a distribution is true concerning all the moments of the form  $\int_{\mathbb{R}^d} \prod_{i=1}^d (x_i^{k_i} \rho(\mathbf{x}) dx_i)$  for all  $k_i \in \mathbb{N}$ . The assertion is no more true when (some of) these moments do not exist and/or dealing only with fractional moments. For

example, this appears for laws that are not exponentially decreasing (e.g. power law such as Lévy noise). This is known as the Hamburger moment problem [30, chap. III, §8]. Finally, moments of various orders often describe fundamental quantities of the involved quantum system [5]. Other similar relationships for particular values of the parameters have also been published [10, 31, 32]. Note also that quantities  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  are insensitive to a stretching factor in the position (or equivalently in the momentum). Moreover, for specific values of  $a$  and/or  $b$ , the moments are linked to physical quantities (e.g. atomic Thomas-Fermi or Dirac exchanges [5]). Thus, it may offer a useful tool to quantify complexity for atomic or chemical systems that can be complementary to those proposed e.g. in [5, 33–35].

In this work we deal with relation (2) and improve it by use of a Rényi-entropy-based approach, in a way similar to the procedure followed by Bialynicki-Birula and Mycielski (BBM in short) [17] and Angulo [28, 29] used to obtain the relations (1) and (2), respectively, from the Shannon entropy. For this purpose we first fix notations and briefly review the entropic uncertainty relations in Section II. Then, in Section III, we find a moment-based formulation of the uncertainty principle which extends and generalizes the relations (1) and (2). In Section IV we carry out a computational analysis of the new moment-based uncertainty relation for hydrogenic and oscillator-like systems, not only because they are the two main quantum prototypes in  $d$ -dimensional physics but also because their position and momentum moments have known analytical expressions in terms of the hyperquantum numbers at all orders [36]. Finally, some conclusions are given in section V. In the appendices we provide help to clearly discuss the proof of the moment uncertainty relation described in Section III.

## II. ENTROPIC UNCERTAINTY RELATIONS: A BRIEF REVIEW

Let us denote by  $\Psi(\mathbf{x})$  and  $\widehat{\Psi}(\mathbf{p})$  the wavefunctions of a  $d$ -dimensional quantum-mechanical system in the position and momentum spaces, respectively, so that

$$\widehat{\Psi}(\mathbf{p}) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \Psi(\mathbf{x}) \exp(-i\mathbf{x}^t \mathbf{p}) d\mathbf{x}$$

where the units with  $\hbar = 1$  are used. The corresponding position and momentum probability densities will be denoted as

$$\rho(\mathbf{x}) = |\Psi(\mathbf{x})|^2 \quad \text{and} \quad \gamma(\mathbf{p}) = |\widehat{\Psi}(\mathbf{p})|^2,$$

respectively. These two density functions are known to be completely characterized by the knowledge of the moments  $\langle r^a \rangle$  and  $\langle p^b \rangle$  of all orders, respectively, where  $r = \|\mathbf{x}\|$  and  $p = \|\mathbf{p}\|$  denote the Euclidean norms of the  $d$ -dimensional position and momentum single-particle operators, respectively. The position expectation value  $\langle f(r) \rangle$  is defined as

$$\langle f(r) \rangle = \int_{\mathbb{R}^d} f(\|\mathbf{x}\|) \rho(\mathbf{x}) d\mathbf{x},$$

and similarly for the expectation value  $\langle f(p) \rangle$  with the momentum density  $\gamma(\mathbf{p})$ .

For notational simplicity, we assume that  $\mathbf{x}$  and  $\mathbf{p}$  have zero mean, so that the variance-based Heisenberg uncertainty relation takes the form (1). Nowadays it is well-known that there exist other uncertainty relations which are much more stringent. They are based on information-theoretic quantities such as the Shannon and Rényi entropies and the Fisher information, which provide complementary measures of the position and momentum probability spreading. Let us here recall the definition of the Rényi entropy of (real) index  $\lambda \geq 0$ ,  $\lambda \neq 1$  [37, 38]

$$H_\lambda(\rho) = \frac{1}{1-\lambda} \log \int_{\mathbb{R}^d} (\rho(\mathbf{x}))^\lambda d\mathbf{x} = \frac{2\lambda}{1-\lambda} \log \|\Psi\|_{2\lambda}, \quad (3)$$

which represents an alternative generalized measure of uncertainty (lack of information) of a random variable with probability density  $\rho = |\Psi|^2$ . Here,  $\|\cdot\|_s$  denotes the  $L^s$  norm for functions:  $\|\Psi\|_p = (\int_{\mathbb{R}^d} |\Psi(\mathbf{x})|^s d\mathbf{x})^{1/s}$ . Note that  $\lim_{\lambda \rightarrow 1} H_\lambda(\rho) = H(\rho) = -\int_{\mathbb{R}^d} \rho(\mathbf{x}) \log \rho(\mathbf{x}) d\mathbf{x}$  is the Shannon entropy, that can thus be viewed as a special case of the family of Rényi entropies (we will write  $H = H_1$ ).

To derive an entropic formulation of the uncertainty relation, the point to start with is the Beckner relation that links the  $L^s$  norm of a (wave) function  $\Psi(\mathbf{x})$  to the  $L^q$  norm of its Fourier transform  $\widehat{\Psi}(\mathbf{p})$  where  $\mathbf{x}$  and  $\mathbf{p}$  are continuous in  $\mathbb{R}^d$ ,  $d$  being the dimension, and  $s$  and  $q$  being conjugated numbers in the Hölder sense:  $1/s + 1/q = 1$ . This relation states that for any  $s \in [1; 2]$  and  $q = s/(1-s)$ :

$$\|\widehat{\Psi}\|_q \leq (C_{s,q})^d \|\Psi\|_s, \quad (4)$$

where

$$C_{s,q} = \left( \frac{2\pi}{s} \right)^{-\frac{1}{2s}} \left( \frac{2\pi}{q} \right)^{\frac{1}{2q}} \quad (5)$$

is the Babenko-Beckner constant. Thus, by taking the logarithm of the relation (4) with  $s = 2\alpha$  and  $q = 2\alpha^*$ , one achieves the relation [18, 19]

$$H_\alpha(\rho) + H_{\alpha^*}(\gamma) \geq d \left( \log(2\pi) + \frac{\log(2\alpha)}{2(\alpha-1)} + \frac{\log(2\alpha^*)}{2(\alpha^*-1)} \right), \quad (6)$$

where  $\alpha$  and  $\alpha^*$  are two real parameters related by  $\frac{1}{\alpha} + \frac{1}{\alpha^*} = 2$ , from which we define  $\alpha^*(\alpha) = \alpha/(2\alpha-1)$ . In principle  $\alpha \in [\frac{1}{2}; 1]$  but it can be seen that by symmetry (exchanging the roles of  $\Psi$  and  $\widehat{\Psi}$ ), this relation holds for any  $\alpha \geq 1/2$ . When  $\alpha \rightarrow 1$ , then  $\alpha^* \rightarrow 1$  and thus the BBM relation [17] dealing with Shannon entropies is recovered

$$H(\rho) + H(\gamma) \geq d(1 + \log(\pi)). \quad (7)$$

The entropic uncertainty relations given in (6) and (7) can be recast in the more convenient product form

$$N_\alpha(\rho)N_{\alpha^*}(\gamma) \geq \mathcal{B}(\alpha), \quad (8)$$

with

$$\mathcal{B}(\alpha) = \frac{\alpha^{\frac{1}{\alpha-1}} \alpha^{*\frac{1}{\alpha^*-1}}}{4e^2} \quad \text{for } \alpha \neq 1 \quad \text{and} \quad \mathcal{B}(1) = \frac{1}{4}, \quad (9)$$

using the so-called Rényi  $\lambda$ -entropy power

$$N_\lambda = \frac{1}{2\pi e} \exp\left(\frac{2}{d} H_\lambda\right), \quad (10)$$

where the limiting case  $\lambda \rightarrow 1$  corresponds to the Shannon entropy power  $N = N_1$ . BBM showed also that his primary relation (7) using Shannon entropies *does imply* the Heisenberg relation (1). To show this, it suffices to search for the maximizer of  $N(\rho)$  under variance constraint  $\langle r^2 \rangle$  fixed, that is known to be a Gaussian of covariance matrix  $\frac{\langle r^2 \rangle}{d} I$  for which the entropy power is  $\frac{\langle r^2 \rangle}{d}$  [38, 39]. The same work is then done (separately) for the momentum, i.e. for  $N(\gamma)$  subject to  $\langle p^2 \rangle$  fixed, to finally achieve

$$\langle r^2 \rangle \langle p^2 \rangle \geq d^2 N(\rho)N(\gamma) \geq \frac{d^2}{4} \quad (11)$$

and thus the Heisenberg relation. Heisenberg inequality is known to be sharp and, fortunately, nothing is lost by this way of making. Indeed, equality between the entropy and its maximal value is reached if and only if  $\rho$  is Gaussian. Furthermore, if (and only if)  $\rho$  is Gaussian,  $\gamma$  is also Gaussian with the “appropriate” variance, and thus simultaneously, in the momentum space the maximum entropy is achieved. In other words, the sum of the maximum entropies corresponds to the maximum of the sum here. Simultaneously, the BBM inequality becomes an equality if and only if  $\rho$  is Gaussian, and thus the succession of inequalities are equalities.

Note now that the relation (8) with Rényi entropies given above concerns only indexes  $\alpha$  and  $\alpha^*$  so that  $2\alpha$  and  $2\alpha^*$  are conjugated in the Hölder sense:  $\frac{1}{2\alpha} + \frac{1}{2\alpha^*} = 1$ . Zozor *et al.*

[20] then showed that the relation (8) extends for *any* pair  $(\alpha, \beta)$  in  $\mathbb{R}_+^2$  such that  $\beta \leq \alpha^*(\alpha)$ , simply noting that  $N_\lambda$  viewed as a function of  $\lambda$  is decreasing (and after decomposing the allowed domain for the parameters into three regions), leading to

$$N_\alpha(\rho)N_\beta(\gamma) \geq \mathcal{Z}(\alpha, \beta) \quad (12)$$

where the bound is

$$\mathcal{Z}(\alpha, \beta) = \begin{cases} 1/e^2 & \text{for } (\alpha, \beta) \in [0; 1/2]^2 \\ \mathcal{B}(\max(\alpha, \beta)) & \text{otherwise} \end{cases} \quad (13)$$

with  $\mathcal{B}$  defined in Eq. (9).

Note that on the “conjugation curve”  $\beta = \alpha^*(\alpha) = \alpha/(2\alpha - 1)$ , the bound is sharp and attained if (and only if)  $\rho$  is Gaussian, since it is the (only) case of equality in the Babenko-Beckner relation (see Lieb’s paper [40]). Finally, let us also mention that Zozor *et al.* [20] showed that for  $\beta > \alpha^*$  no uncertainty principle exists, in the sense that the product of Rényi entropy powers is just trivially non-negative. But below the conjugation curve, it is not known yet neither the sharpest bound, nor the states that saturate the uncertainty relation.

### III. THE MOMENT-BASED UNCERTAINTY RELATION

The uncertainty relation (2) based on the moments  $\langle r^a \rangle$  and  $\langle p^b \rangle$  was obtained in [28, 29, 41] by use of two elements: the Shannon-entropy-based BBM relation (7) and the maximizer [41] of the Shannon entropy of the position (momentum) density subject to (s.t.) the constraint  $\langle r^a \rangle$  (resp.  $\langle p^b \rangle$ ). Let us remark that such a bound cannot be sharp. If we denote by  $\Psi_{\max,a}$  the wavefunction that gives the maximizer of  $N(\rho)$  s.t.  $\langle r^a \rangle$  and by  $\tilde{\Psi}_{\max,b}$  the wavefunction that maximizes  $N(\gamma)$  s.t.  $\langle p^b \rangle$ , then these two functions are not linked by a Fourier transformation, namely  $\tilde{\Psi}_{\max,b} \neq \hat{\Psi}_{\max,a}$ , except for the particular case  $a = b = 2$ . Or, in other words, the sum of the maximal entropies is not here the maximum of the sum. When deriving the Heisenberg relation from the Bialynicki-Birula relation, although the maximization is made separately on each Shannon entropy, it appears that the squared roots of the two maximizers are precisely linked by a Fourier transformation. Without entering into details here, let us consider the example of  $\rho_{\max,a} = \arg \max H(\rho)$  s.t.  $\langle r^a \rangle$  that

is a generalized Gaussian of index  $a$  [42, 43]. Its squared root is thus a generalized Gaussian of index  $a/2$  and the Fourier transform of the probability density function (pdf) is not a generalized Gaussian (i.e. not the maximizer of the other Shannon entropy): it is linked to an  $\alpha$ -stable law of stability index  $a/2$  [44].

In this Section we improve the relation (2) in a similar way but using the Rényi entropy (3), which includes the Shannon entropy as a particular case. Our procedure has the following steps:

1. Start with the Rényi-entropy-based inequality (12), namely  $N_\alpha(\rho)N_\beta(\gamma) \geq \mathcal{Z}(\alpha, \beta)$ , with the bound  $\mathcal{Z}$  defined in Eq. (13).
2. Search for the maximum Rényi entropy power  $N_\alpha(\rho)$  s.t.  $\langle r^a \rangle$ . This will give rise to a relation of the form  $\langle r^a \rangle^{2/a} \geq N_\alpha(\rho)\mathcal{M}(a, \alpha)$ , where the bound  $\mathcal{M}$  has to be obtained in terms of  $a$  and  $\alpha$  (see Appendices A and B).
3. Similarly (and separately) for the momentum one will arrive at the relation  $\langle p^b \rangle^{2/b} \geq N_\beta(\gamma)\mathcal{M}(b, \beta)$
4. These will lead to  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geq N_\alpha(\rho)N_\beta(\gamma)\mathcal{M}(a, \alpha)\mathcal{M}(b, \beta) \geq \mathcal{M}(a, \alpha)\mathcal{M}(b, \beta)\mathcal{Z}(\alpha, \beta)$ , for every pair  $(a, b) \in \mathbb{R}_+^2$ .
5. Finally, the best bound we can find is  $\mathcal{C}(a, b) = \max_{\alpha, \beta} \mathcal{M}(a, \alpha)\mathcal{M}(b, \beta)\mathcal{Z}(\alpha, \beta)$ , where  $\beta \leq \alpha^*(\alpha)$  (other restrictions come out that considerably reduce the  $(\alpha, \beta)$  domain for searching the maximum; see Appendix C).

It can be shown (see Appendix C 1) that the desired maximum is *on* the conjugation curve  $\beta = \alpha^*(\alpha)$ , and then  $\mathcal{C}(a, b) = \max_{\alpha} \mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*)\mathcal{B}(\alpha)$ .

As previously mentioned, the bound must be at least the same as the case of Dehesa *et al.* [5], since the latter corresponds to the particular situation  $\alpha = \beta = 1$  in our computations.

The main result of the present effort is summarized here (and proved in the appendices): For any  $a \geq b > 0$  there exists an Uncertainty Principle that can be stated in the following way for arbitrary-order moments of the position and momentum observables in  $d$ -dimensional systems

$$\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geq \mathcal{C}(a, b) = \max_{\alpha \in D} \mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*), \quad (14)$$

where  $\mathcal{B}(\alpha)$  is defined in Eq. (9),  $\alpha^* = \alpha/(2\alpha - 1)$ ,

$$D = \left[ \max \left( \frac{1}{2}, \frac{d}{d+a} \right); 1 \right], \quad (15)$$

and the function  $\mathcal{M}$  has the form

$$\mathcal{M}(l, \lambda) = \begin{cases} 2\pi e \left( \frac{l}{\Omega B \left( \frac{d}{l}, 1 - \frac{\lambda}{\lambda-1} - \frac{d}{l} \right)} \right)^{\frac{2}{d}} \left( \frac{-d(\lambda-1)}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{l}} \left( \frac{l\lambda}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{d(\lambda-1)}}, & 1 - \frac{l}{l+d} < \lambda < 1 \\ 2\pi e \left( \frac{l}{\Omega \Gamma \left( \frac{d}{l} \right)} \right)^{\frac{2}{d}} \left( \frac{d}{le} \right)^{\frac{2}{l}}, & \lambda = 1 \\ 2\pi e \left( \frac{l}{\Omega B \left( \frac{d}{l}, \frac{\lambda}{\lambda-1} \right)} \right)^{\frac{2}{d}} \left( \frac{d(\lambda-1)}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{\lambda}} \left( \frac{l\lambda}{d(\lambda-1) + l\lambda} \right)^{\frac{2}{d(\lambda-1)}}, & \lambda > 1 \end{cases} \quad (16)$$

with  $\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)}$  and  $B(x, y)$  the beta function.

The case  $b \geq a > 0$  can be treated using the symmetry (proved in the appendix),

$$\alpha_{\text{opt}}(a, b) = \arg \max_{\alpha \in D} \mathcal{B}(\alpha) \mathcal{M}(a, \alpha) \mathcal{M}(b, \alpha^*) \quad (17)$$

satisfies

$$\alpha_{\text{opt}}(b, a) = (\alpha_{\text{opt}}(a, b))^*, \quad (18)$$

and then

$$\mathcal{C}(b, a) = \mathcal{C}(a, b). \quad (19)$$

The symmetry on  $\alpha_{\text{opt}}$  allows also to conclude that  $\alpha_{\text{opt}}(a, a) = 1$  and thus the optimal bound from our approach coincides with that of Angulo, given in (2). Unfortunately, except for the case  $a = b$ , we have not been able yet to obtain an analytical expression for  $\mathcal{C}(a, b)$ .

Figure 1 depicts the bound  $\mathcal{C}(a, b)$  for given values of  $a$ , as a function of  $b$ , compared to the bound  $\mathcal{D}(a, b)$ . From the figure we see that the bound is substantially improved when  $b \neq a$ , especially as  $b$  departs considerably from  $a$ .

Figure 2 depicts the optimal  $\alpha = \alpha_{\text{opt}}$  as a function of  $b$  in the same configurations as in Fig. 1. The curves illustrate that only for  $a = b$ , the optimal bound is obtained for  $\alpha_{\text{opt}} = 1$ . For  $a \neq b$ , a finer study of  $\mathcal{M}$  could allow to even reduce the domain  $D$  where  $\alpha_{\text{opt}}$  lies.

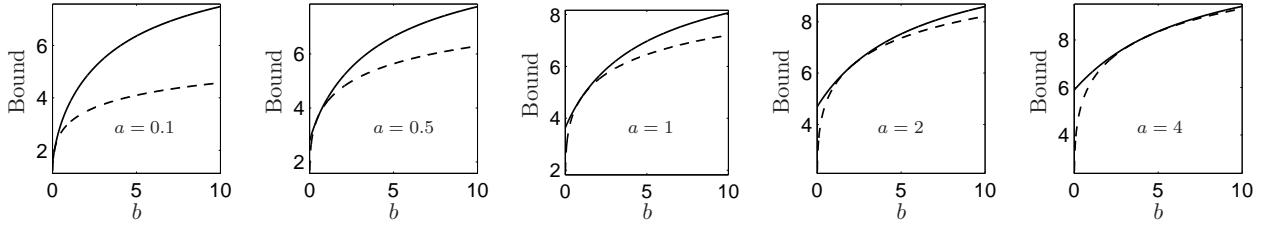


FIG. 1. Bound  $\mathcal{C}(a, b)$  (solid line) given in (14) compared to  $\mathcal{D}(a, b)$  in (2) (dashed line), versus  $b$ , for given  $a = 0.1, 0.5, 1, 2$  and  $4$  respectively, with  $d = 5$ . For each value of  $a$ , the new bound  $\mathcal{C}$  is always above  $\mathcal{D}$ ; both functions coincide when  $b = a$ .

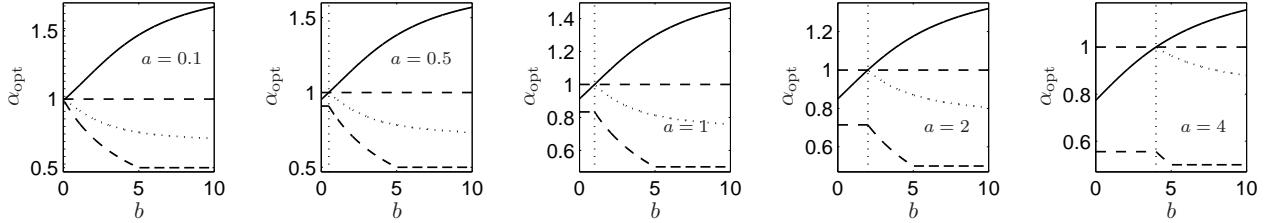


FIG. 2.  $\alpha_{\text{opt}}(a, b)$  (solid line) given in (17), versus  $b$ , for given  $a = 0.1, 0.5, 1, 2$  and  $4$  respectively, with  $d = 5$ . The dotted vertical line indicates  $b = a$ . Thus, left to this line,  $a \geq b > 0$  and  $\alpha_{\text{opt}}$  has to be searched in  $D$  Eq. (15). This domain is indicated by the dashed lines. At the opposite, right to the vertical dotted line,  $b > a$ . Thus, symmetry Eq. (18) is used and  $\alpha_{\text{opt}}(b, a) = (\alpha_{\text{opt}}(a, b))^*$  is seek. Since  $b > a > 0$ , this parameter is also in domain  $D$  Eq. (15) (where  $b$  replaces  $a$ ); the dotted curve represents  $\alpha_{\text{opt}}(b, a)$  (the solid curve being  $\alpha_{\text{opt}}(a, b)$ ) and domain  $D$  is still represented by the dashed lines.

#### IV. APPLICATION TO CENTRAL POTENTIAL PROBLEMS

Let us now apply and discuss the minimal uncertainty bound (14) for the two main prototypes of  $d$ -dimensional physics: hydrogenic and oscillator-like systems. But before, let us give a brief review on eigensolutions for quantum systems in central potentials.

### A. Eigensolutions for central potentials: a brief review

In both hydrogenic and oscillator cases, the quantum systems are described by the physical solutions of the Schrödinger equation

$$\left[ -\frac{1}{2} \nabla^2 + V(r) \right] \Psi = E \Psi, \quad (20)$$

where  $V(r)$  is a radial potential and where, without loss of generality, the mass is set to  $m = 1$ . It is well known [45] that the wavefunctions of a Hamiltonian with central potential can be separated out into a radial,  $R_{E,l}(r)$ , and an angular,  $\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})$ , part as

$$\Psi_{E,\{\mu\}}(\mathbf{x}) = R_{E,l}(r) \mathcal{Y}_{\{\mu\}}(\Omega_{d-1}). \quad (21)$$

The position  $\mathbf{x} = (x_1, \dots, x_d)$  is given in hyperspherical coordinates as  $(r, \theta_1, \theta_2, \dots, \theta_{d-1}) \equiv (r, \Omega_{d-1})$ , where naturally  $\|\mathbf{x}\| = r = \sqrt{\sum_{i=1}^d x_i^2} \in [0; +\infty)$  and  $x_i = r \left( \prod_{k=1}^{i-1} \sin \theta_k \right) \cos \theta_i$  for  $1 \leq i \leq d$  and with  $\theta_i \in [0; \pi], i < d-1, \theta_{d-1} \in [0; 2\pi]$ . By convention  $\theta_d = 0$  and the empty product is the unity. The angular part, common to any central potential, is given by the hyperspherical harmonics [45, 46]  $\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})$ , which are known to satisfy the eigenvalue equation

$$\Lambda_{d-1}^2 \mathcal{Y}_{\{\mu\}}(\Omega_{d-1}) = l(l+d-2) \mathcal{Y}_{\{\mu\}}(\Omega_{d-1}),$$

associated to the generalized angular momentum operator given by

$$\Lambda_{d-1}^2 = - \sum_{i=1}^{d-1} \frac{(\sin \theta_i)^{i+1-d}}{\left( \prod_{j=1}^{i-1} \sin \theta_j \right)^2} \frac{\partial}{\partial \theta_i} \left[ (\sin \theta_i)^{d-i-1} \frac{\partial}{\partial \theta_i} \right].$$

The angular quantum numbers  $\{\mu\} = \{\mu_1 \equiv l, \mu_2, \dots, \mu_{d-1} \equiv m\}$  characterize the hyperspherical harmonics, and satisfy the chain of inequalities  $l \equiv \mu_1 \geq \mu_2 \geq \dots \geq \mu_{d-2} \geq |\mu_{d-1}| \equiv |m|$ .

The radial part  $R_{E,l}(r)$  fulfills the second-order differential equation

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} - \frac{d-1}{2r} \frac{d}{dr} + \frac{l(l+d-2)}{2r^2} + V(r) \right] R_{E,l}(r) = E R_{E,l}(r),$$

which only depends on the eigenenergy  $E$ , the dimensionality  $d$  and the largest angular quantum number  $l = \mu_1$ .

Then, the quantum-mechanical position probability density for central systems is given by

$$\rho_{E,\{\mu\}}(\mathbf{x}) = |\Psi_{E,\{\mu\}}(\mathbf{x})|^2 = |R_{E,l}(r)|^2 |\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})|^2. \quad (22)$$

It is worth remarking that this density function is normalized to unity. Let us bring here that

$$\int_0^{+\infty} r^{d-1} |R_{E,l}(r)|^2 dr = 1 \quad \text{and} \quad \int_{[0;\pi)^{d-2} \times [0:2\pi)} |\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})|^2 d\Omega_{d-1} = 1,$$

and that the volume element can be expressed in hyperspherical coordinates as

$$d\mathbf{x} = r^{d-1} dr d\Omega_{d-1} = r^{d-1} dr \left( \prod_{j=1}^{d-2} (\sin \theta_j)^{d-j-1} d\theta_j \right) d\theta_{d-1}.$$

Thus, the moment  $\langle r^a \rangle$  for the  $d$ -dimensional density  $\rho_{E,\{\mu\}}(\mathbf{x})$  has the expression

$$\langle r^a \rangle = \int_0^{+\infty} r^{d+a-1} |R_{E,l}(r)|^2 dr, \quad (23)$$

which is only characterized by the position radial wavefunction  $R_{E,l}(r)$  of the particle.

From the Fourier transform of  $\Psi_{E,\{\mu\}}$ , it comes out that in the momentum domain the wavefunction  $\widehat{\Psi}_{E,\{\mu\}}$  also separates under the form

$$\widehat{\Psi}_{E,\{\mu\}}(\mathbf{p}) = M_{E,l}(p) \mathcal{Y}_{\{\mu\}}(\Omega_{d-1}).$$

(see e.g. [36, 46, 47]) with the same hyperspherical part, and the radial part expresses from  $R_{E,l}$  through the Hankel transform (e.g. [48, 49]),

$$M_{E,l}(p) = p^{1-\frac{d}{2}} \int_0^{+\infty} r^{\frac{d}{2}} R_{E,l}(r) J_{l+\frac{d}{2}-1}(pr) dr \quad (24)$$

( $J_\nu$  is the Bessel function of the first kind and of order  $\nu$ ). Immediately, in the momentum space, the moment  $\langle p^b \rangle$  has the expression

$$\langle p^b \rangle = \int_0^{+\infty} p^{d+b-1} |M_{E,l}(p)|^2 dp, \quad (25)$$

which is only characterized by the momentum radial wavefunction  $M_{E,l}(p)$  of the particle.

These expressions have allowed to find numerous information-theoretic properties [24, 25, 36, 45, 50, 51] of general central potentials, particularly the Heisenberg [25] and Fisher-information [24, 25] uncertainty relations, as recently reviewed [5].

## B. Application to $d$ -dimensional hydrogenic systems

Let us now examine the accuracy of the moments-based uncertainty relations (14) for the main prototype of  $d$ -dimensional systems, namely the hydrogenic atom. This system

has been recently investigated in Ref. [36] in full detail from the information theory point of view. In this case, the potential has the form  $V(r) = -\frac{1}{r}$  (without loss of generality, the atomic number  $Z$  is taken to be 1) and the energies are

$$E = -\frac{1}{2\eta^2}, \quad \eta = n + \frac{d-3}{2}, \quad n = 1, 2, \dots$$

where  $\eta$  denotes the grand principal quantum number. The radial part of the eigenfunctions are thus completely calculable [36, 50, 51]. The radial wavefunction in position domain expresses as

$$R_{E,l}(r) = \left(\frac{\eta}{2}\right)^{\frac{d}{2}} \sqrt{\frac{\Gamma(\eta - L)}{2\eta\Gamma(\eta + L + 1)}} \tilde{r}^{L - \frac{d-3}{2}} \exp\left(-\frac{\tilde{r}}{2}\right) \mathcal{L}_{\eta-L-1}^{2L+1}(\tilde{r}) \quad (26)$$

where  $L = l + \frac{d-3}{2}$ ,  $l = 0, \dots, n-1$  is the grand orbital quantum number,  $\tilde{r} = \frac{2r}{\eta}$  is a reduced (dimensionless) position and  $\mathcal{L}_p^q$  are the Laguerre polynomials. As it is shown in Refs. [36, 50, 51], after the Hankel transform (24), the radial wavefunction in momentum domain expresses as

$$M_{E,l}(p) = 2^{2L+3} \sqrt{\frac{\Gamma(\eta - L)}{2\pi\Gamma(\eta + L + 1)}} \Gamma(L + 1) \eta^{\frac{d+1}{2}} \frac{\tilde{p}^l}{(1 + \tilde{p}^2)^{L+2}} \mathcal{G}_{\eta-L-1}^{L+1}\left(\frac{1 - \tilde{p}^2}{1 + \tilde{p}^2}\right)$$

where  $\tilde{p} = \eta p$  is a reduced (dimensionless) momentum and  $\mathcal{G}_p^q$  are the Gegenbauer polynomials. From these expressions together with (23) and (25), it is shown [36] that the position and momentum moments of arbitrary orders, corresponding to a given eigenstate characterized by an energy  $E$  and an angular quantum number  $l$  (or equivalently by  $\eta$  and  $L$ ) have the expressions:

$$\langle r^a \rangle = \frac{\eta^{a-1}\Gamma(2L+a+3)}{2^{a+1}\Gamma(2L+2)} {}_3F_2(-\eta + L + 1, -a - 1, a + 2; 2L + 2, 1; 1)$$

and

$$\begin{aligned} \langle p^b \rangle &= \frac{4\Gamma(\eta + L + 1)\Gamma(L + \frac{b+3}{2})\Gamma(L + \frac{5-b}{2})}{\eta^{b-1}\Gamma(\eta - L)\Gamma^2(L + \frac{3}{2})\Gamma(2L + 4)} \times \\ &{}_5F_4\left(L - \eta + 1, L + \eta + 1, L + 1, L + \frac{b+3}{2}, L + \frac{5-b}{2}; 2L + 2, L + \frac{3}{2}, L + 2, L + \frac{5}{2}; 1\right) \end{aligned} \quad (27)$$

for  $b < 2L + 5$ , where  ${}_pF_q$  are the generalized hypergeometric functions (see e.g. [52, 2.19.14-15] and reflective properties of hypergeometric functions). Note that the momentum wave

function is not exponentially decreasing. The direct consequence is that not all moments exist in the momentum domain, what is reflected in the restriction for the values of  $b$ .

Thus, the uncertainty product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  can be computed and therefore studied analytically for hydrogenic systems in  $d$ -dimensions. As an illustration, Fig. 3 depicts the product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  computed from (27), for  $(a, b) = (1, 2)$  and Fig. 4 plots the case  $(a, b) = (1, 4)$  (both for  $d = 3$ ) when the system is in the state  $(E, l)$ , together with the corresponding bound  $\mathcal{C}(a, b)$  given in (14)–(16).

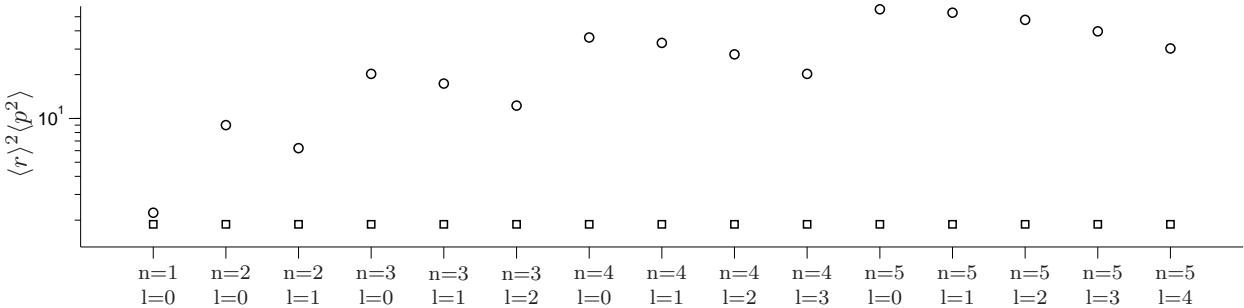


FIG. 3. Product  $\langle r \rangle^2 \langle p^2 \rangle$ , i.e.  $(a, b) = (1, 2)$  in eqs. (27) (circles) for the lowest energy states and lower bound  $\mathcal{C}(1, 2)$ , eqs. (14)–(16), of this product (squares), for 3-dimensional hydrogenic systems ( $d = 3$ ).

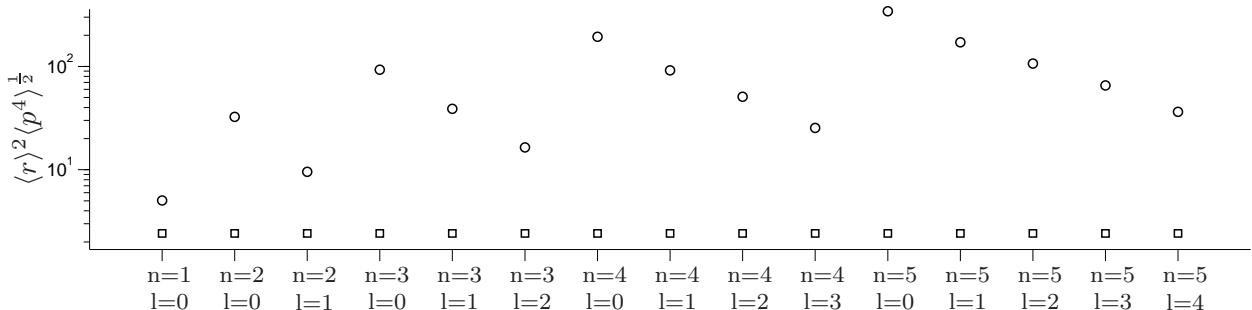


FIG. 4. Product  $\langle r \rangle^2 \langle p^4 \rangle^{\frac{1}{2}}$ , i.e.  $(a, b) = (1, 4)$  in eqs. (27) (circles) for the lowest energy states and lower bound  $\mathcal{C}(1, 4)$ , eqs. (14)–(16), of this product (squares), for 3-dimensional hydrogenic systems ( $d = 3$ ).

We can see from both figures that, although not sharp, the bound  $\mathcal{C}(a, b)$  is close to the product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  for the ground state ( $n = 1$  and  $l = 0$ ). However, when  $n$  increases, the discrepancy from the bound increases (and decreases with  $l$  for fixed  $n$ ). The same behavior

occurs for other pairs  $(a, b)$  whatever the dimensionality  $d$ . Since hydrogenic systems belong to the family of radial potential systems, this suggests that a refinement can be found in the context of radial systems as already done for the usual variance-based Heisenberg inequality, and for Fisher information-based versions [24, 25]. To give a further illustration, Fig. 5 depicts  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  as a function of  $b$ , for fixed  $a$ , and for the ground state ( $n = 1$ ,  $l = 0$ ) in 3 dimensions. In all the cases shown, we observe the existence of a value of  $b$  that is “optimum” in the sense that the uncertainty product is close to the bound proposed here, corresponding to a situation of low generalized uncertainty. As  $b$  increases (up to  $2L+5 = 5$  for the ground state in 3 dimensions), the uncertainty departs from our bound. Finally, one observes for the tested values of  $a$  that the lower bound has a concave behavior versus  $b$ , while the product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  exhibits a convex behavior. This suggests the existence of an optimal value of  $b$  (function of  $a$ ) in terms of low discrepancy from the bound.

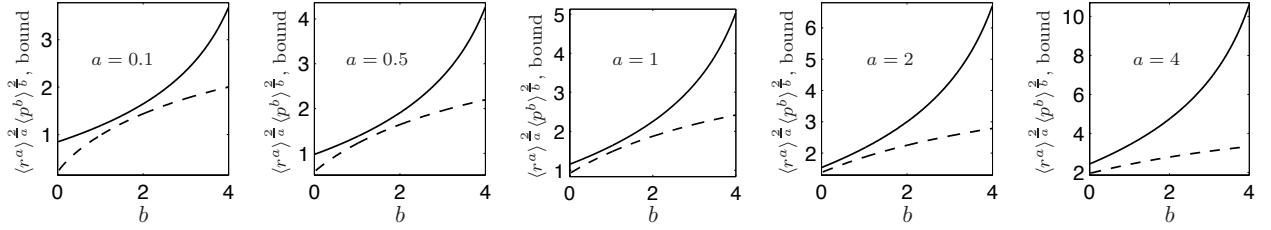


FIG. 5. Product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  (solid lines) in the ground state ( $n = 1$ ,  $l = 0$ ), for fixed  $a = 0.1$ ,  $a = 0.5$ ,  $a = 1$ ,  $a = 2$  and  $a = 4$  respectively, and lower bound (dashed lines) for 3-dimensional hydrogenic systems ( $d = 3$ ).

### C. Application to $d$ -dimensional oscillator-like systems

Let us consider now a potential of the form  $V(r) = \frac{1}{2}r^2$  (without loss of generality, the product mass squared pulsation is taken as  $m\omega^2 = 1$ ). In this case, the energies are

$$E = 2n + l + \frac{d}{2}, \quad n = 0, 1, \dots \quad \text{and} \quad l = 0, 1, \dots$$

and the radial parts of the wavefunctions are again known [53]. They express as

$$R_{E,l}(r) = \sqrt{\frac{2\Gamma(n+1)}{\Gamma(n+l+d/2)}} r^l \exp\left(-\frac{r^2}{2}\right) \mathcal{L}_n^{l+d/2-1}(r^2) \quad (28)$$

and  $M_{E,l}(p) = R_{E,l}(p)$ . Comparing (28) with (26), after a change of variables  $\tilde{r} = r^2$ , one can easily show from (27) that the statistical moments write down as

$$\langle r^a \rangle = \frac{\Gamma(l + \frac{d+a}{2})}{\Gamma(l + \frac{d}{2})} {}_3F_2 \left( -n, -\frac{a}{2}, \frac{a}{2} + 1; L + \frac{d}{2}, 1; 1 \right)$$

and (29)

$$\langle p^b \rangle = \frac{\Gamma(l + \frac{d+b}{2})}{\Gamma(l + \frac{d}{2})} {}_3F_2 \left( -n, -\frac{b}{2}, \frac{b}{2} + 1; L + \frac{d}{2}, 1; 1 \right)$$

(see also Ref. [54] for special cases).

Figure 6 describes the moments product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  using (29), for  $(a, b) = (1, 2)$  and Fig. 7 exhibits the case  $(a, b) = (1, 4)$  (both for  $d = 3$ ), together with the corresponding bound  $\mathcal{C}(a, b)$  given in (14)–(16).

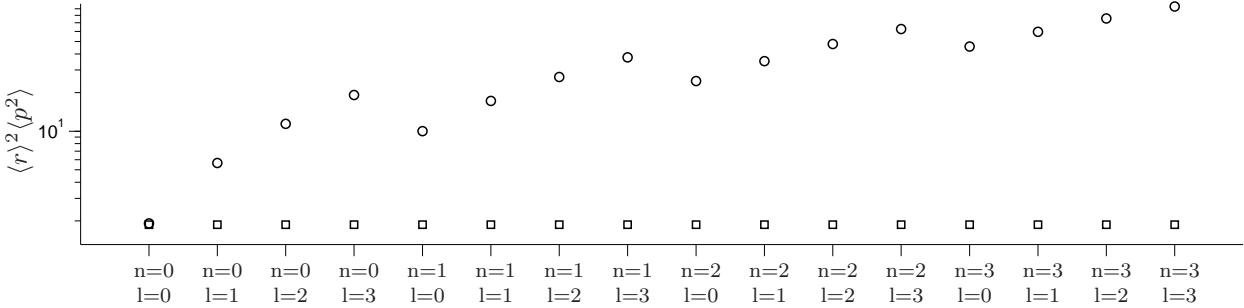


FIG. 6. Product  $\langle r \rangle^2 \langle p^2 \rangle$ , i.e.  $(a, b) = (1, 2)$  in eqs. (27) (circles) for the lowest energy states and lower bound  $\mathcal{C}(1, 2)$ , eqs. (14)–(16), of this product (squares) for 3-dimensional harmonic oscillators ( $d = 3$ ).

We can see from these figures also that even if not sharp, the bound  $\mathcal{C}(a, b)$  is very close to the product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$ , for the ground state ( $n = 0$  and  $l = 0$ ). The global behavior is similar to what happens for the hydrogenic systems: there is a discrepancy from the bound as  $n$  increases. But here, the discrepancy increases also with  $l$  when  $n$  is fixed. The same behavior occurs for other pairs  $(a, b)$  and whatever the dimension  $d$ . In fact, when observing more finely  $\langle r \rangle^2 \langle p^2 \rangle$  and  $\langle r \rangle^2 \langle p^4 \rangle^{\frac{1}{2}}$ , it appears that these products essentially depend on the energy level, i.e the values of these products for a fixed value of  $2n + l$  are very close (see e.g.  $n = 0, l = 2$  or  $n = 1, l = 0$ ). This was true also for the hydrogenic systems, but it is strongly more pronounced for the harmonic oscillator. All these observations reinforce our

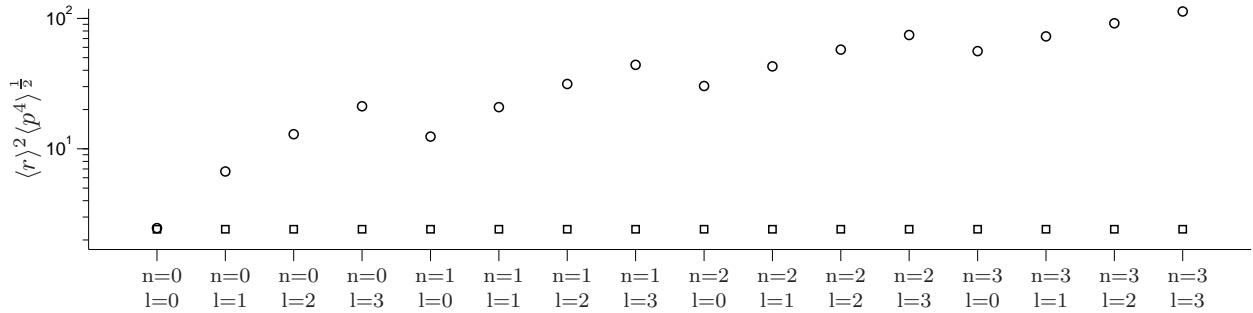


FIG. 7. Product  $\langle r \rangle^2 \langle p^4 \rangle^{\frac{1}{2}}$ , i.e.  $(a, b) = (1, 4)$  in eqs. (27) (circles) for the lowest energy states and lower bound  $\mathcal{C}(1, 4)$ , eqs. (14)–(16), of this product (squares) for 3-dimensional harmonic oscillators ( $d = 3$ ).

“conjecture” that refinement can be found in the context of radial systems, for moments’ orders other than  $a = b = 2$ , at least in terms of energy levels.

A further illustration is given by Fig. 8 where  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  versus  $b$  is depicted, for different fixed values of  $a$ , in the case of the ground state ( $n = 0, l = 0$ ).

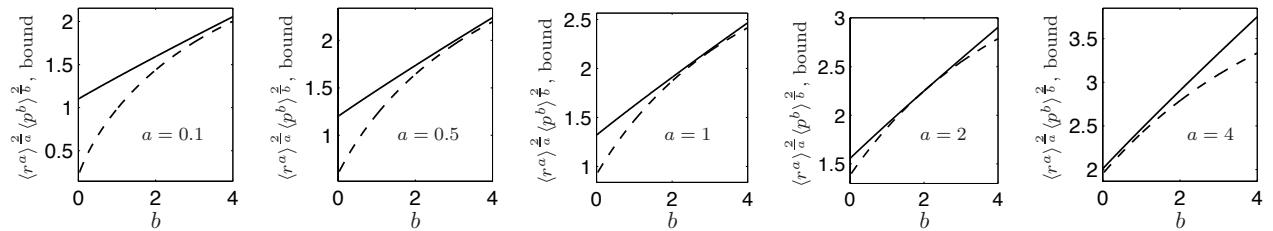


FIG. 8. Product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  (solid lines) in the ground state ( $n = 0, l = 0$ ), for fixed  $a = 0.1, a = 0.5, a = 1, a = 2$  and  $a = 4$  respectively, and lower bound (dashed lines) for 3-dimensional oscillators ( $d = 3$ ).

Globally the behavior of the moments’ product compared to the bound observed here is similar to that of the hydrogenic systems. However, the discrepancy from the bound is less pronounced for the harmonic oscillator (in the ground state) than for the hydrogen systems. Note that the bound is achieved in the case when  $a = b = 2$ . This case corresponds to the classical variance-based Heisenberg inequality. Moreover, the ground state of the oscillator leads to the Gaussian pdf  $\rho$  (and  $\gamma$ ): in this case the variance-based Heisenberg inequality is saturated. One can again observe the convexity of the product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  (in fact almost linear): together with the observed concavity of the lower bound, this reinforce

our conjecture on the existence of an optimal value of  $b(a)$  in terms of low discrepancy from the bound. This remains to be studied more systematically and more deeply.

## V. DISCUSSION AND CONCLUSIONS

In this paper we have proposed an improved version of the moment-based mathematical formulation of the position–momentum uncertainty principle for quantum systems that generalizes the seminal variance-based formulation of Heisenberg. The main result of this contribution is formalized in Eq. (14) together with eqs. (15), (16) and (9):  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geq \mathcal{C}(a, b)$ . In contrast to the entropic uncertainty relations (like Eq. (12)), the new formulation is based on spreading measures which describe physical observables. Our present approach suffers, however, from the fact that the lower bound  $\mathcal{C}(a, b)$  found here for the product of the position and momentum moments for arbitrary  $a$  and  $b$  is not sharp. To tackle this issue a variational approach may be envisaged, although it is a difficult task. Another alternative might be to employ appropriate Sobolev-like inequalities, as done for entropic formulations (see e.g. Ref. [17–19, 21]).

The new moment-based uncertainty relation is physico-computationally analyzed in some  $d$ -dimensional quantum systems. Precisely, the bound of the moment-based uncertainty relation is compared to the product of the moments for hydrogenic and oscillator-like systems. In both cases analytic expressions of the moments exist in terms of hypergeometric functions (eqs. (27) and (29) respectively). Our results suggest that the improvement of this relation for general central potentials seems possible whatever the orders  $a$  and  $b$  of the moments, at least in terms of energy levels. Such an improvement exists in the variance-based context  $a = b = 2$  [24, 25], but for moments of arbitrary order this issue is a fully open problem which deserves to be variationally solved for both fundamental and applied reasons. This suggests also that the product  $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$  can be envisaged as a useful tool to quantify the complexity and organization of various physical systems. However, the properties of such a complexity measure should be analyzed in more detail.

## ACKNOWLEDGMENTS

S.Z. and M.P. are grateful to the CNRS (France) and CONICET (Argentina) for the cooperation grant that partially enabled this work. M.P. also acknowledges financial support by CONICET and ANPCyT. P.S.-M. and J.S.D. are very grateful to Junta de Andalucía (Spain) for the grants FQM-2445 and FQM-4643, and the Ministerio de Ciencia e Innovación (Spain) for the grant FIS2008-02380.

## Appendix A: Evaluation of the maximizers of the Rényi entropy power under moment constraint

In section III (steps 2 and 3) we established the necessity of searching for the maximum of the Rényi entropy power  $N_\alpha(\rho)$  subjected to given moment  $\langle r^a \rangle$  and  $N_\beta(\gamma)$  s.t.  $\langle p^b \rangle$ . This variational problem has been tackled and partially solved by Dehesa *et al.* [55]. Similarly to what is done for variance constraint, the problem is to maximize the frequency entropic moment of order  $\lambda > 0$ , an increasing function of the entropy power,  $\int_{\mathbb{R}^d} f(\mathbf{x})^\lambda d\mathbf{x}$  s.t.  $\int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} = 1$  and  $\int_{\mathbb{R}^d} \|\mathbf{x}\|^l f(\mathbf{x}) d\mathbf{x} = \langle r^l \rangle$ , with  $l > 0$  and where  $\|\mathbf{x}\| = r$  is the Euclidean norm of  $\mathbf{x}$ . Note that we work here with the variables  $\mathbf{x}$  and  $r$ , but the results obtained will be valid in the momentum domain, changing  $\mathbf{x}$  to  $\mathbf{p}$  and  $r$  to  $p$ . Then, we have to maximize  $\int_{\mathbb{R}^d} (f(\mathbf{x})^\lambda - \mu f(\mathbf{x}) - \nu \|\mathbf{x}\|^l f(\mathbf{x})) d\mathbf{x}$ , where  $\mu$  and  $\nu$  are the Lagrange factors. From the corresponding Euler–Lagrange equation, one obtains that  $f$  must be of the form  $f(\mathbf{x}) = \left(\frac{\mu+\nu\|\mathbf{x}\|^l}{\lambda}\right)_+^{\frac{1}{\lambda-1}}$ , where  $(y)_+ = \max(y, 0)$ . With integrability arguments ( $f$  must be a pdf, and thus positive and integrable),  $\mu > 0$  and  $\nu$  must have the sign of  $1 - \lambda$ , and thus the pdf that maximizes the entropy power  $N_\lambda$  s.t.  $\langle r^l \rangle$  can be recast under the form

$$f_{\lambda,l}(\mathbf{x}) = C \left(1 - (\lambda - 1)(\|\mathbf{x}\|/\delta)^l\right)_+^{\frac{1}{\lambda-1}}. \quad (\text{A1})$$

This pdf is sometimes called generalized Gaussian [56, 57], but this terminology is not adequate. Indeed, when  $\lambda \rightarrow 1$ , this pdf tends to  $f_{1,l}(\mathbf{x}) = C \exp(-\|\mathbf{x}/\delta\|^l)$  that is also sometimes named generalized Gaussian (or also Kotz-type) [43, 58, 59] (and also sometimes as stretched exponential or power exponential [59, 60]). Furthermore, when  $l = 2$  one can recognize in (A1) the well known  $q$ -Gaussian (also known as Student-t or Student-r depending on the sign of  $1 - \lambda$ ), where  $q = 2 - \lambda$  and thus the generalization (A1) is known

under the terminology of *stretched  $q$ -exponential* [55, 61] or even *generalized  $q$ -Gaussian* of parameter  $q = 2 - \lambda$  and (stretching) parameter  $l$ .

Constants  $C$  and  $\delta$  are to be determined so that the constraints are satisfied. The normalization constraint reads

$$\begin{aligned} 1 &= C \int_{\mathbb{R}^d} \left(1 - (\lambda - 1)(\|\mathbf{x}\|/\delta)^l\right)_+^{\frac{1}{\lambda-1}} d\mathbf{x} \\ &= C \Omega \int_0^{+\infty} r^{d-1} \left(1 - (\lambda - 1)(r/\delta)^l\right)_+^{\frac{1}{\lambda-1}} dr \\ &= \frac{C \Omega \delta^d}{l|\lambda - 1|^{d/l}} \int_0^{+\infty} t^{d/l-1} (1 - \text{sign}(\lambda - 1) t)_+^{\frac{1}{\lambda-1}} dt \end{aligned}$$

where the second line comes from [62, Eq. 4.642], with  $\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)}$  that is the surface of the  $d$ -dimensional unit sphere and where the third line comes from the change of variable  $r = \delta(t/|1 - \lambda|)^{1/l}$ . The integral term, that we will denote  $B_1(l, \lambda)$ , expresses via the beta function  $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$ , from [62, Eq. 8.380-1 & 8.380-3], one finally obtains

$$1 = \frac{C \Omega \delta^d}{l|\lambda - 1|^{d/l}} B_1(l, \lambda) \quad (\text{A2})$$

where

$$B_1(l, \lambda) = \begin{cases} B\left(\frac{d}{l}, \frac{\lambda}{\lambda-1}\right) & \text{if } \lambda > 1 \\ B\left(\frac{d}{l}, 1 + \frac{\lambda}{1-\lambda} - \frac{d}{l}\right) & \text{if } 1 - \frac{l}{d} < \lambda < 1 \end{cases} \quad (\text{A3})$$

Indeed, the integral converges provided that  $\lambda > 1 - l/d$ .

In the same vein, the power moment constraint writes

$$\begin{aligned} \langle r^l \rangle &= C \int_{\mathbb{R}^d} \|\mathbf{x}\|^l \left(1 - (\lambda - 1)(\|\mathbf{x}\|/\delta)^l\right)_+^{\frac{1}{\lambda-1}} d\mathbf{x} \\ &= C \Omega \int_0^{+\infty} r^{l+d-1} \left(1 - (\lambda - 1)(r/\delta)^l\right)_+^{\frac{1}{\lambda-1}} dr \\ &= \frac{C \Omega \delta^{l+d}}{l|\lambda - 1|^{d/l+1}} \int_0^{+\infty} t^{d/l} (1 - \text{sign}(\lambda - 1) t)_+^{\frac{1}{\lambda-1}} dt \end{aligned}$$

where the integral term, denoted here  $B_m(l, \lambda)$ , expresses via the beta function from [62, Eq. 8.380-1 & 8.380-3], leading to

$$\langle r^l \rangle = \frac{C \Omega \delta^{l+d}}{l|\lambda - 1|^{d/l+1}} B_m(l, \lambda) \quad (\text{A4})$$

where

$$B_m(l, \lambda) = \begin{cases} B\left(\frac{d}{l} + 1, \frac{\lambda}{\lambda-1}\right) & \text{if } \lambda > 1 \\ B\left(\frac{d}{l} + 1, \frac{\lambda}{1-\lambda} - \frac{d}{l}\right) & \text{if } 1 - \frac{l}{d+l} < \lambda < 1 \end{cases} \quad (\text{A5})$$

Note that the existence of the latter integral implies a stronger restriction to  $\lambda$  than the one coming from the normalization, that is we require now:

$$\lambda > 1 - \frac{l}{d+l} = \frac{d}{d+l}. \quad (\text{A6})$$

In both constraints, the case  $\lambda = 1$  can be recovered by letting  $\lambda \rightarrow 1^+$  or  $\lambda \rightarrow 1^-$  (from [63, 6.1.47] or [62, 8.328-1],  $\lim_{y \rightarrow \infty} B(x, y)x^y = \Gamma(x)$ ): it is not needed to treat this case separately.

## Appendix B: Maximal entropy power $N_\lambda$ and bound for the moment $\langle r^l \rangle$

Following the procedure proposed in section III, we discuss here the bounds for the moments  $\langle r^a \rangle$  and  $\langle p^b \rangle$ . From (A1), the maximal  $\lambda$ -norm of  $f_{\lambda,l}(\mathbf{x})$  to the power  $\lambda$  takes the form

$$\begin{aligned} \|f_{\lambda,l}\|_\lambda^\lambda &= C^\lambda \int_{\mathbb{R}^d} (1 - (\lambda - 1)(\|\mathbf{x}\|/\delta)^l)_+^{\frac{\lambda}{\lambda-1}} d\mathbf{x} \\ &= C^\lambda \Omega \int_0^{+\infty} r^{d-1} (1 - (\lambda - 1)(r/\delta)^l)_+^{\frac{\lambda}{\lambda-1}} dr \\ &= \frac{C^\lambda \Omega \delta^d}{l|\lambda - 1|^{d/l}} \int_0^{+\infty} t^{d/l-1} (1 - \text{sign}(\lambda - 1) t)_+^{\frac{\lambda}{\lambda-1}} dt. \end{aligned}$$

Then, from [62, Eq. 8.380-1 & 8.380-3] we obtain

$$\|f_{\lambda,l}\|_\lambda^\lambda = \frac{C^\lambda \Omega \delta^d}{l|\lambda - 1|^{d/l}} B_h(l, \lambda), \quad (\text{B1})$$

where we have defined

$$B_h(l, \lambda) = \begin{cases} B\left(\frac{d}{l}, \frac{\lambda}{\lambda-1} + 1\right) & \text{if } \lambda > 1 \\ B\left(\frac{d}{l}, \frac{\lambda}{1-\lambda} - \frac{d}{l}\right) & \text{if } 1 - \frac{l}{d+l} < \lambda < 1 \end{cases} \quad (\text{B2})$$

that adds no new restriction on  $\lambda$ . Thus, the maximal value of the Rényi entropy power is

$$\begin{aligned}
N_\lambda(f_{\lambda,l}) &= \frac{1}{2\pi e} \left( \|f\|_\lambda^{\frac{\lambda}{1-\lambda}} \right)^{\frac{2}{d}} \\
&= \frac{1}{2\pi e} \left( C^{\frac{\lambda}{1-\lambda}} \left( \frac{\Omega \delta^d}{l|\lambda-1|^{d/l}} \right)^{\frac{1}{1-\lambda}} B_h^{\frac{1}{1-\lambda}} \right)^{\frac{2}{d}} \\
&= \frac{1}{2\pi e} \left( C^{-1} \left( \frac{C \Omega \delta^d}{l|\lambda-1|^{d/l}} B_1 \right)^{\frac{1}{1-\lambda}} \left( \frac{B_h}{B_1} \right)^{\frac{1}{1-\lambda}} \right)^{\frac{2}{d}} \\
&= \frac{1}{2\pi e} \left( C^{-1} \left( \frac{B_h}{B_1} \right)^{\frac{1}{1-\lambda}} \right)^{\frac{2}{d}}
\end{aligned}$$

from (A2) and where the arguments of  $B_1$  and  $B_h$  are omitted for simplicity. Taking the ratio  $\frac{\langle r^l \rangle^{d/l}}{1^{d/l+1}}$  from (A2) and (A4), one obtains

$$C^{-1} = \frac{\Omega}{l} B_1 \left( \frac{B_1}{B_m} \right)^{d/l} \langle r^l \rangle^{d/l},$$

that gives

$$N_\lambda(f_{\lambda,l}) = \frac{1}{2\pi e} \left( \frac{\Omega B_1}{l} \left( \frac{B_1}{B_m} \right)^{d/l} \left( \frac{B_h}{B_1} \right)^{\frac{1}{1-\lambda}} \langle r^l \rangle^{d/l} \right)^{\frac{2}{d}}.$$

One can simplify a little bit this expression by considering the parameter

$$\mu = \mu(\lambda) = \frac{\lambda}{\lambda-1} \tag{B3}$$

that governs the maximal entropy power, with  $\mu > 1$  or  $\mu < -d/l$ . Noting that

$$\frac{B_1}{B_m} = \text{sign}(\mu) \frac{d+l\mu}{d} \quad \text{and} \quad \frac{B_h}{B_1} = \frac{l\mu}{d+l\mu} \tag{B4}$$

so that

$$N_\lambda(f_{\lambda,l}) = \frac{1}{2\pi e} \left( \frac{\Omega B_1(l, \lambda)}{l} \left( \frac{d+l\mu}{\text{sign}(\mu) d} \right)^{\frac{d}{l}} \left( \frac{d+l\mu}{l\mu} \right)^{\mu-1} \langle r^l \rangle^{d/l} \right)^{\frac{2}{d}}. \tag{B5}$$

We finally obtain that the Rényi entropy power of any pdf  $\rho$ ,  $N_\lambda(\rho) = \frac{1}{2\pi e} \left( \|\rho\|_\lambda^{\frac{\lambda}{1-\lambda}} \right)^{\frac{2}{d}}$ , s.t. fixed  $\langle r^l \rangle$ , is bounded from above by the maximum value  $N_\lambda(f_{\lambda,l})$ . Therefore we can write

$$\langle r^l \rangle^{2/l} \geq N_\lambda(\rho) \mathcal{M}(l, \lambda) \tag{B6}$$

where function  $\mathcal{M}$  expresses as

$$\mathcal{M}(l, \lambda) = \begin{cases} 2\pi e \left( \frac{l}{\Omega B \left( \frac{d}{l}, \mu \right)} \right)^{\frac{2}{d}} \left( \frac{d}{d + l\mu} \right)^{\frac{2}{l}} \left( \frac{l\mu}{d + l\mu} \right)^{\frac{2(\mu-1)}{d}} & \text{if } \lambda > 1 \\ 2\pi e \left( \frac{l}{\Omega \Gamma \left( \frac{d}{l} \right)} \right)^{\frac{2}{d}} \left( \frac{d}{l e} \right)^{\frac{2}{l}} & \text{if } \lambda = 1 \\ 2\pi e \left( \frac{l}{\Omega B \left( \frac{d}{l}, 1 - \mu - \frac{d}{l} \right)} \right)^{\frac{2}{d}} \left( -\frac{d}{d + l\mu} \right)^{\frac{2}{l}} \left( \frac{l\mu}{d + l\mu} \right)^{\frac{2(\mu-1)}{d}} & \text{if } 1 - \frac{l}{l+d} < \lambda < 1 \end{cases} \quad (B7)$$

with

$$\mu = \frac{\lambda}{\lambda - 1} \quad (B8)$$

and where  $\mathcal{M}(l, 1) = \lim_{\lambda \rightarrow 1} \mathcal{M}(l, \lambda)$  from the first and/or second expression of  $\mathcal{M}$  and [63, 6.1.41].

### Appendix C: Generalized Heisenberg-like uncertainty relation

Using (B6) applied to  $r$  with  $l = a$  and  $\lambda = \alpha$  and applied to  $p$  with  $l = b$  and  $\lambda = \beta$  respectively, and using (12), we achieve the relation established in point 4 of section III

$$\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geq \mathcal{Z}(\alpha, \beta) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta) \quad (C1)$$

for all  $a, b > 0$ ,  $\alpha > \frac{d}{d+a}$ ,  $\beta > \frac{d}{d+b}$ ,  $\beta \leq \frac{\alpha}{2\alpha-1}$  and with the bounds  $\mathcal{Z}$  and  $\mathcal{B}$  given in eqs. (13) and (B7).

#### 1. The maximal bound is on the conjugation curve $\beta = \alpha^*$

We will now show that the pair  $(\alpha, \beta)$  that maximizes  $\mathcal{Z}(\alpha, \beta) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta)$  is on the conjugation curve, namely for  $\beta = \alpha^* = \alpha/(2\alpha - 1)$ , for any values of  $a$  and  $b$  (under the existence condition for  $\mathcal{M}$ ).

#### a. Function $\mathcal{M}(l, \lambda)$ is increasing with $\lambda$

Let us first consider the derivative of  $\mathcal{M}(l, \lambda)$  versus  $\lambda$ .

For  $\lambda > 1$ , i.e.  $\mu = \frac{\lambda}{\lambda-1} > 1$ ,

$$\begin{aligned}\frac{\partial}{\partial \mu} \log \mathcal{M} &= \frac{\partial}{\partial \mu} \left( -\frac{2}{d} \log \Gamma(\mu) + \frac{2}{d} \log \Gamma \left( \mu + \frac{d}{l} \right) - \frac{2}{l} \log(d + l\mu) + \frac{2(\mu-1)}{d} \log \left( \frac{l\mu}{d+l\mu} \right) \right) \\ &= \frac{2}{d} \left( -\psi(\mu) + \psi \left( \mu + \frac{d}{l} \right) + \frac{l}{d+l\mu} - \frac{1}{\mu} + \log \left( \frac{l\mu}{d+l\mu} \right) \right)\end{aligned}$$

where  $\psi(x) = \frac{d}{dx} \log \Gamma(x)$  is the digamma function.

Similarly, for  $\lambda \in (1 - \frac{l}{l+d}; 1)$ , i.e.  $\mu < -d/l$ ,

$$\begin{aligned}\frac{\partial}{\partial \mu} \log \mathcal{M} &= \frac{\partial}{\partial \mu} \left( -\frac{2}{d} \log \Gamma \left( 1 - \mu - \frac{d}{l} \right) + \frac{2}{d} \log \Gamma(1 - \mu) \right. \\ &\quad \left. - \frac{2}{l} \log(-d - l\mu) + \frac{2(\mu-1)}{d} \log \left( \frac{l\mu}{d+l\mu} \right) \right) \\ &= \frac{2}{d} \left( -\psi(1 - \mu) + \psi \left( 1 - \mu - \frac{d}{l} \right) + \frac{l}{d+l\mu} - \frac{1}{\mu} + \log \left( \frac{l\mu}{d+l\mu} \right) \right) \\ &= \frac{2}{d} \left( \psi \left( -\frac{d+l\mu}{l} \right) - \psi(-\mu) + \log \left( \frac{l\mu}{d+l\mu} \right) \right)\end{aligned}$$

the last simplification coming from [62, Eq. 8.365-1].

To summarize, noting that  $\partial \mu / \partial \lambda = -1/(\lambda - 1)^2$ ,

$$\left\{ \begin{array}{ll} \frac{\partial}{\partial \lambda} \log \mathcal{M}(l, \lambda) &= \frac{2}{d(\lambda-1)^2} \left( \psi(\mu) + \frac{1}{\mu} - \log \mu \right. \\ &\quad \left. - \psi \left( \mu + \frac{d}{l} \right) - \frac{1}{\mu + \frac{d}{l}} + \log \left( \mu + \frac{d}{l} \right) \right) & \text{if } \lambda > 1 \\ \frac{\partial}{\partial \lambda} \log \mathcal{M}(l, \lambda) &= \frac{2}{d(\lambda-1)^2} \left( \psi(-\mu) - \log(-\mu) \right. \\ &\quad \left. - \psi \left( -\mu - \frac{d}{l} \right) + \log \left( -\mu - \frac{d}{l} \right) \right) & \text{if } 1 - \frac{l}{l+d} < \lambda < 1 \end{array} \right. \quad (C2)$$

Taking the limit  $\lambda \rightarrow 1^+$  from the first line, or  $\lambda \rightarrow 1^-$  from the second line, and  $\mathcal{M}$  being continuous in  $\lambda = 1$ , we achieve  $\frac{\partial}{\partial \lambda} \log \mathcal{M}(l, \lambda) \big|_{\lambda=1} = \frac{1}{l}$ .

Let us consider now the terms in the parentheses in the right-hand side of the first line in Eq. (C2). They can be written as  $g(\mu) - g(\mu + d/l)$  with,

$$g(\mu) = \psi(\mu) + \frac{1}{\mu} - \log \mu. \quad (C3)$$

Then, from [63, 6.4.1]

$$\begin{aligned}
g'(\mu) &= \psi'(\mu) - \frac{1}{\mu} - \frac{1}{\mu^2} \\
&= \int_0^{+\infty} \frac{t}{1-e^{-t}} e^{-\mu t} dt - \int_0^{+\infty} e^{-\mu t} dt - \int_0^{+\infty} t e^{-\mu t} dt \\
&= \int_0^{+\infty} \frac{-1 + e^{-t} + t e^{-t}}{1-e^{-t}} e^{-\mu t} dt.
\end{aligned}$$

Now, it is easy to show that  $-1 + e^{-t} + t e^{-t} \leq 0$  for  $t \geq 0$  that permits to conclude that  $g' \leq 0$  and thus that  $g$  is decreasing. As a conclusion,  $g(\mu) - g(\mu + d/l) \geq 0$  and thus  $\frac{\partial}{\partial \lambda} \log \mathcal{M} \geq 0$ :  $\mathcal{M}$  is increasing in  $(1; +\infty)$ .

Similarly, the terms in parentheses in the right-hand side of second line ( $\mu < -d/l < 0$  here), writes  $h(\mu) - h(\mu + d/l)$  with,

$$h(\mu) = \psi(-\mu) - \log(-\mu)$$

and give from [63, 6.4.1]

$$\begin{aligned}
h'(\mu) &= -\psi'(-\mu) - \frac{1}{\mu} \\
&= \int_0^{+\infty} \frac{-t}{1-e^{-t}} e^{\mu t} dt + \int_0^{+\infty} e^{\mu t} dt \\
&= \int_0^{+\infty} \frac{1-t-e^{-t}}{1-e^{-t}} e^{\mu t} dt.
\end{aligned}$$

Then, it is easy to show that  $1-t-e^{-t} \leq 0$  for  $t \geq 0$  that permits to conclude that  $h' \leq 0$  and thus that  $h$  is decreasing. As a conclusion,  $h(\mu) - h(\mu + d/l) \geq 0$  and thus also for  $\lambda \in (1 - \frac{l}{l+d}; 1)$  we have  $\frac{\partial}{\partial \lambda} \log \mathcal{M} \geq 0$ :  $\mathcal{M}$  is increasing.

*b.  $\mathcal{B}(\lambda)$  increases with  $\lambda \in [1/2; 1]$  and decreases with  $\lambda > 1$*

From (9) and  $\lambda^* = \lambda/(2\lambda - 1)$ , the derivative of  $\mathcal{B}(\lambda)$  writes

$$\begin{aligned}
\frac{\partial}{\partial \lambda} \log \mathcal{B}(\lambda) &= \frac{\partial}{\partial \lambda} \left( \frac{\log \lambda}{\lambda - 1} + \frac{\log \lambda^*}{\lambda^* - 1} \right) \\
&= \frac{\partial}{\partial \lambda} \left( \frac{\log \lambda}{\lambda - 1} \right) + \frac{\partial}{\partial \lambda^*} \left( \frac{\log \lambda^*}{\lambda^* - 1} \right) \frac{\partial \lambda^*}{\partial \lambda} \\
&= \left( \frac{1}{\lambda(\lambda - 1)} - \frac{\log \lambda}{(\lambda - 1)^2} \right) - \left( \frac{1}{\lambda^*(\lambda^* - 1)} - \frac{\log \lambda^*}{(\lambda^* - 1)^2} \right) \frac{1}{(2\lambda - 1)^2}
\end{aligned}$$

that is

$$\frac{\partial}{\partial \lambda} \log \mathcal{B}(\lambda) = \frac{1}{(\lambda - 1)^2} \left( 2 - \frac{2}{\lambda} - \log(2\lambda - 1) \right). \quad (\text{C4})$$

A short study of the right hand side, show that this quantity is positive if  $\lambda \in [1/2 ; 1]$  and negative if  $\lambda \geq 1$ :  $\mathcal{B}$  increases with  $\lambda$  in  $[1/2 ; 1]$  and then decreases for larger values of  $\lambda$ .

c. *Domain where the maximal bound has to be searched*

Remind that starting from (C1), namely  $\langle r^a \rangle_a^{\frac{2}{a}} \langle p^b \rangle_b^{\frac{2}{b}} \geq \mathcal{Z}(\alpha, \beta) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta)$ , the best bound is then so that  $\mathcal{Z}(\alpha, \beta) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta)$  is maximized as a function of  $\alpha$  and  $\beta$ . Let us now consider the following sets in the  $(\alpha, \beta)$  plane:

$$\left\{ \begin{array}{l} D_\alpha = \{(\alpha, \beta) \in \mathbb{R}_+^2 \mid \alpha \geq 1, \beta \leq \alpha^*\} \\ D_\beta = \{(\alpha, \beta) \in \mathbb{R}_+^2 \mid \beta \geq 1, \alpha \leq \beta^*\} \\ S_\alpha = \{(\alpha, \beta) \in [0 ; 1]^2 \mid \beta \leq \alpha\} \\ S_\beta = \{(\alpha, \beta) \in [0 ; 1]^2 \mid \alpha \leq \beta\} \\ S_1 = S_\alpha \cup S_\beta \end{array} \right.$$

where  $\alpha^* = \frac{\alpha}{2\alpha-1}$  and  $\beta^* = \frac{\beta}{2\beta-1}$ . These sets are represented in Fig. 9.

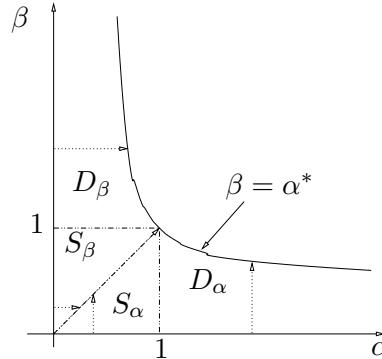


FIG. 9. Sets  $D_\alpha$ ,  $D_\beta$ ,  $S_\alpha$  and  $S_\beta$  in the plane  $(\alpha, \beta)$ . The solid curve represents the pairs of conjugated parameters, i.e.  $\beta = \alpha^*$ . The dotted arrows indicate that  $\mathcal{Z}(\alpha, \beta) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta)$  increases when the pair  $(\alpha, \beta)$  moves along their directions, in the sets where they are plotted.

In order to study the best bound, we consider each subset:

- We first consider domain  $D_\alpha$  and fix  $\alpha$ . From Eq. (13), the bound is then  $\mathcal{Z}(\alpha, \beta) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta) = \mathcal{B}(\alpha) \mathcal{M}(a, \alpha) \mathcal{M}(b, \beta)$  and from the previous study of  $\mathcal{M}$  we can know that it increases with  $\beta$ . Thus, the bound is maximum precisely *on* the conjugation curve  $\beta = \alpha^*$ .

- By symmetry, in domain  $D_\beta$  and fixing  $\beta$ , one shows again that the bound is maximal on the conjugation curve  $\alpha = \beta^*$ .
- In the domain  $S_1$  we discuss the following cases:
  - The maximum bound must be achieved on the line segment  $\alpha = \beta$ . Indeed, in  $S_\alpha$ , the bound is given by  $\mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \beta)$  if  $\alpha \geq 1/2$  and  $\mathcal{M}(a, \alpha)\mathcal{M}(b, \beta)/e^2$  otherwise. Again, fixing  $\alpha$ , the bound is increasing with  $\beta$  and thus is maximum for  $\beta = \alpha$ . This remains valid, by symmetry, in  $S_\beta$ , and thus in all  $S_1$ .
  - For  $\alpha \leq 1/2$ , on the line segment  $\alpha = \beta$  the bound is  $\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha)/e^2$  and thus increases with  $\alpha$ : it is maximum for  $\alpha = 1/2$ .
  - For  $\alpha \in (1/2 ; 1]$ , the bound expresses  $\mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha)$  and tends to  $\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha)/e^2$  for  $\alpha \rightarrow 1/2$ .  $\mathcal{B}$  being an increasing function in  $[1/2 ; 1]$  and since  $\mathcal{M}$  is increasing, the bound is then maximum for  $\alpha = 1$ .

As a conclusion, on  $S_1$  the maximum bound is achieved when  $\alpha = \beta = 1$  that is again *on the conjugation curve*.

## 2. Maximal bound and properties

The best bound of the generalized Heisenberg relation one can achieve by our approach is then

$$\mathcal{C}(a, b) = \max_{\alpha \in D(a, b)} \mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*) \quad (\text{C5})$$

where the domain of search  $D$  is ruled by the restriction on the domain of existence of  $\mathcal{M}$ . We will come back later on this domain.

### a. Symmetries

Let us denote by  $\alpha_{\text{opt}}(a, b)$  the index that leads to  $\mathcal{C}(a, b)$ , i.e.

$$\alpha_{\text{opt}}(a, b) = \arg \max_{\alpha} \mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*) \quad (\text{C6})$$

Noticing that  $\mathcal{B}(\alpha) = \mathcal{B}(\alpha^*)$ , one immediately observes from (C6) that

$$\begin{cases} \mathcal{C}(b, a) &= \mathcal{C}(a, b) \\ \alpha_{\text{opt}}(b, a) &= (\alpha_{\text{opt}}(a, b))^*. \end{cases} \quad (\text{C7})$$

Thus, without loss of generality, one can restrict the study to the case with  $a \geq b$ .

*b. Reduced domain of search*

Consider the situation where  $a \geq b$ .

If  $\alpha > 1$ , then  $\alpha^* < 1$ . We will show that the bound  $\mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*)$  decreases with  $\alpha$ ; thus the maximum must satisfy  $\alpha \leq 1$ .

We have already seen that  $\mathcal{B}(\alpha)$  decreases when  $\alpha > 1$ . Consider then the part  $\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*)$ . Remembering that  $\alpha^* = \frac{\alpha}{2\alpha-1}$ , one has  $\frac{\partial \alpha^*}{\partial \alpha} = -\frac{1}{(2\alpha-1)^2}$ . Moreover, one has  $\frac{1}{(\alpha^*-1)^2} = \frac{(2\alpha-1)^2}{(\alpha-1)^2}$  and  $\mu(\alpha^*) = \frac{\alpha^*}{\alpha^*-1} = -\frac{\alpha}{\alpha-1} = -\mu(\alpha)$  from Eq. (B3). Then, from (C2),

$$\begin{aligned} \frac{\partial}{\partial \alpha} \log(\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*)) &= \frac{\partial}{\partial \alpha} \log \mathcal{M}(a, \alpha) + \frac{\partial \alpha^*}{\partial \alpha} \frac{\partial}{\partial \alpha^*} \log \mathcal{M}(b, \alpha^*) \\ &= \frac{2}{d(\alpha-1)^2} \left( \frac{1}{\mu} - \frac{1}{\mu+d_a} - \psi(\mu+d_a) + \psi(\mu-d_b) + \log(\mu+d_a) - \log(\mu-d_b) \right) \end{aligned}$$

where  $\mu$  stands for  $\mu(\alpha)$ ,  $d_a = d/a$  and  $d_b = d/b$ . The goal is then to show the negativity of

$$k(\mu, d_a, d_b) = \frac{1}{\mu} - \frac{1}{\mu+d_a} - \psi(\mu+d_a) + \log(\mu+d_a) + \psi(\mu-d_b) - \log(\mu-d_b) \quad (\text{C8})$$

keeping in mind that  $d_a \leq d_b$ . To this end, we can view this function in terms of  $d_a$  for instance, and thus the sense of variation of  $k(\mu, d_a, d_b) = -g(\mu+d_a) + g(\mu-d_b) + 1/\mu - 1/(\mu-d_b)$  is the same than the sense of variation of  $-g(\mu+d_a) = -\psi(\mu+d_a) - \frac{1}{\mu+d_a} + \log(\mu+d_a)$  introduced Eq. (C3), versus  $d_a$ . We have shown that function  $g$  is decreasing and thus  $k$  is increasing with  $d_a$ . Since,  $d_a \leq d_b$ , to show that  $k$  is negative, it is then sufficient to show that  $k(\mu, d_b, d_b)$  is negative. From [63, 6.4.1]

$$\begin{aligned} \frac{\partial k(\mu, d_b, d_b)}{\partial d_b} &= \frac{1}{\mu+d_b} + \frac{1}{(\mu+d_b)^2} - \psi'(\mu+d_b) + \frac{1}{\mu-d_b} - \psi'(\mu-d_b) \\ &= \int_0^{+\infty} \left[ \left( 1 + t - \frac{t}{1-e^{-t}} \right) e^{-d_b t} + \left( 1 - \frac{t}{1-e^{-t}} \right) e^{+d_b t} \right] e^{-\mu t} dt \\ &= \int_0^{+\infty} \left[ (1 - e^{-t} - t e^{-t}) e^{-d_b t} + (1 - t - e^{-t}) e^{+d_b t} \right] \frac{e^{-\mu t}}{1-e^{-t}} dt. \end{aligned}$$

Now, it is quite easy to show that the term in square brackets is decreasing with  $d_b$  since the derivative in  $d_b$  is negative (the factors of  $e^{\pm d_b t}$  are negative). For  $d_b = 0$ , it is no more hard to show that the square bracket is negative, that permits to conclude that for any  $d_b$  the square bracket term is negative:  $k(\mu, d_b, d_b)$  decreases with  $d_b$ .

At last  $k(\mu, 0, 0) = 0$  and thus  $k(\mu, d_b, d_b) \leq 0$ , implying that for any  $d_a \leq d_b$  one has  $k(\mu, d_a, d_b) \leq 0$ .

As claimed,  $\frac{\partial}{\partial \alpha} \log (\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*)) \leq 0$  for  $\alpha > 1$ . Together with the decrease of  $\mathcal{B}$  when  $\alpha > 1$  we conclude that the maximum of  $\mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*)$  is attained for  $\alpha < 1$ .

To finish to determine the domain of search for the maximal bound, when  $a \geq b$ , implies that  $\alpha \leq 1$  as just found,  $\alpha > 1/2$  since it must be on the conjugation curve, and from (C2),  $\alpha > \frac{d}{d+a}$ .

In summary, for  $a \geq b$ ,

$$\mathcal{C}(a, b) = \max_{\alpha \in (\max(\frac{1}{2}, \frac{d}{d+a}), 1]} \mathcal{B}(\alpha)\mathcal{M}(a, \alpha)\mathcal{M}(b, \alpha^*) \quad (\text{C9})$$

where  $\mathcal{B}$  and  $\mathcal{M}$  are respectively given by (9) and (B7).

- [1] W. C. Price and S. S. Chissick (Eds.), *The Uncertainty Principle and Foundations of Quantum Mechanics* (Wiley, New-York, 1977).
- [2] A. I. Miller (Ed.), *Sixty-Two Years of Uncertainty: historical, philosophical, and physical inquiries into the foundations of quantum mechanics* (Plenum Press, New-York, 1990).
- [3] D. R. Herschbach and J. Avery and O Goscinski (Eds.), *Dimensional Scaling in Chemical Physics* (Springer Verlag, New-York, 2001).
- [4] E. Lieb and W. Thirring (Ed.), *The Stability of Matter: From Atoms to Stars, Selecta of E. H. Lieb* (Springer Verlag, Berlin, 2002).
- [5] J. S. Dehesa, S. López-Rosa, and D. Manzano, in *Statistical Complexities: Application to Electronic Structure*, edited by K. D. Sen (Springer, Berlin, 2010).
- [6] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
- [7] V. Vedral, *Introduction to Quantum Information Science* (Oxford University Press, Oxford, 2006).
- [8] W. Heisenberg, *Zeitschrift für Physik A* **43**, 172 (1927).
- [9] E. H. Kennard, *Zeitschrift für Physik* **44**, 326 (1927).
- [10] G. B. Folland and A. Sitaram, *Journal of Fourier Analysis and Applications* **3**, 207 (1997).

- [11] P. Busch, T. Heinonen, and P. Lahti, Physics Reports **452**, 155 (2007).
- [12] I. Bialynicki-Birula and L. Rudnicki, (2010), arxiv:1001.4668v1 [quant-ph].
- [13] D. Deutsch, Physical Review Letters **50**, 631 (1983).
- [14] J. B. M. Uffink and J. Hilgevoord, Foundations in Physics **15**, 925 (1985).
- [15] J. B. M. Uffink, *Measures of Uncertainty and the Uncertainty Principle*, Ph.D. thesis, University of Utrecht, Utrecht, The Netherlands (1990), see also references therein.
- [16] J. Hilgevoord and J. B. M. Uffink, in *Proceedings of the International Conference on Microphysical Reality and Quantum Description*, Vol. 1, edited by F. Selleri, A. van der Merwe, and G. Tarozzi (Reidal, Dordrecht: Kluwer, (Urbino, Italia, 1985), 1988) pp. 91–114.
- [17] I. Bialynicki-Birula and J. Mycielski, Communications in Mathematical Physics **44**, 129 (1975).
- [18] I. Bialynicki-Birula, Physical Review A **74**, 052101 (2006).
- [19] S. Zozor and C. Vignat, Physica A **375**, 499 (2007).
- [20] S. Zozor, M. Portesi, and C. Vignat, Physica A **387**, 4800 (2008).
- [21] A. K. Rajagopal, Physics Letters A **205**, 32 (1995).
- [22] M. Portesi and A. Plastino, Physica A **225**, 412 (1996).
- [23] H. Maassen and J. B. M. Uffink, Physical Review Letters **60**, 1103 (1988).
- [24] E. Romera, P. Sánchez-Moreno, and J. S. Dehesa, Journal of Mathematical Physics **47**, 103504 (2006).
- [25] P. Sánchez-Moreno, R. González-Férez, and J. S. Dehesa, New Journal of Physics **8**, 330 (2006).
- [26] P. Sánchez-Moreno, A. R. Plastino, and J. S. Dehesa, (2010), preprint.
- [27] S. Wehner and A. Winter, New Journal of Physics **12**, 025009 (2010).
- [28] J. C. Angulo, Journal of Physics A **26**, 6493 (1993).
- [29] J. C. Angulo, Physical Review A **50**, 311 (1994).
- [30] D. V. Widder, *The Laplace Transform*, Princeton Mathematical Series (Princeton University Press, 1946).
- [31] E. Romera, J. C. Angulo, and J. S. Dehesa, Physical Review A **59**, 4064 (1999).
- [32] Y. A. Wang and E. A. Carter, Physical Review A **60**, 4153 (1999).
- [33] R. López-Ruiz, H. L. Mancini, and X. Calbet, Physics Letters A **209**, 321 (1995).
- [34] S. López-Rosa, J. C. Angulo, and J. Antolín, Physica A **388**, 2081 (2009).

[35] S. López-Rosa, R. O. Esquivel, J. C. Angulo, J. Antolín, J. S. Dehesa, and N. Flores-Gallegos, *Journal of Chemical Theory and Computation* **6**, 145 (2010).

[36] J. S. Dehesa, S. López-Rosa, A. Martínez-Finkelshtein, and R. J. Yáñez, *International Journal of Quantum Chemistry* **110**, 1529 (2010).

[37] A. Rényi, in *Proceeding of the 4th Berkeley Symposium on Mathematical Statistics and Probability* **1**, 547 (1961).

[38] T. M. Cover and J. A. Thomas, *Elements of Information Theory* (John Wiley & Sons, New-York, 1991).

[39] J. A. Costa, A. O. Hero III, and C. Vignat, in *4th International Workshop on Energy Minimization Methods in Computer Vision and Pattern Recognition (EMMCVPR)*, Lecture Notes in Computer Sciences, Vol. 2683, edited by A. Rangarajan, M. A. T. Figueiredo, and J. Zerubia (Springer Verlag, Lisbon, Portugal, 2003) pp. 211–226.

[40] E. H. Lieb, *Inventiones Mathematicae* **102**, 179 (1990).

[41] J. C. Angulo and J. S. Dehesa, *Journal of Chemical Physics* **97**, 6485 (1992).

[42] S. Nadarajah, *Journal of Applied Statistics* **32**, 685 (2005).

[43] M. K. Varanasi and B. Aazhang, *Journal of Acoustical Society of America* **86**, 1404 (1989).

[44] S. Zozor and C. Vignat, *IEEE transactions on Signal Processing* **58**, 134 (2010).

[45] R. J. Yáñez, W. Van Assche, R. González-Férez, and J. Sánchez-Dehesa, *Journal of Mathematical Physics* **40**, 5675 (1999).

[46] J. S. Avery, *Hyperspherical Harmonics and Generalized Sturmians* (Kluwer Academic, Dordrecht, 2002).

[47] R. J. Yáñez, W. Van Assche, and J. S. Dehesa, *Physical Review A* **50**, 3065 (1994).

[48] R. Lord, *Biometrika* **41**, 44 (1954).

[49] J. S. Avery, *Journal of Computational and Applied Mathematics* **233**, 1366 (2010).

[50] W. Van Assche, R. J. Yáñez, R. González-Férez, and J. S. Dehesa, *Journal of Mathematical Physics* **41**, 6600 (2000).

[51] V. F. Tarasov, *International Journal of Modern Physics B* **18**, 3177 (2004).

[52] A. P. Prudnikov, Y. A. Brychkov, and O. I. Marichev, *Intergals and Series*, Vol. 2: Special Functions (Gordon and Breach Science Publishers, New-York, 1986).

[53] J. D. Louck and W. H. Shaffer, *Journal of Molecular Spectroscopy* **4**, 298 (1960).

[54] J. D. Louck and W. H. Shaffer, *Journal of Molecular Spectroscopy* **4**, 334 (1960).

- [55] J. S. Dehesa, F. J. Galvez, and I. Porras, *Physical Review A* **40**, 35 (1989).
- [56] C. Tsallis, R. M. Mendes, and A. R. Plastino, *Physica A* **261**, 534 (1998).
- [57] A. Andai, *Journal of Multivariate Analysis* **100**, 777 (2009).
- [58] S. Kotz and S. Nadarajah, *Statistics and Probability Letters* **54**, 171 (2001).
- [59] Y. Kano, *Journal of Multivariate Analysis* **51**, 139 (1994).
- [60] T. J. Kozubowski, *Statistics* **36**, 219 (2002).
- [61] C. Tsallis and E. K. Lenzi, *Chemical Physics* **284**, 341 (2002).
- [62] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, 7th ed. (Academic Press, San Diego, 2007).
- [63] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, 9th printing (Dover, New-York, 1970).